

Course Code	Course Name	Credits
26CH110	FUNDAMENTALS OF AI IN CHEMISTRY	04

Course Objectives

- To understand the fundamental concepts of Artificial Intelligence (AI) and its relevance in chemistry.
- To explore the applications of AI in chemical sciences, including data analysis, drug discovery, and materials science.
- To develop awareness of the role of AI in solving environmental and real-world chemical problems.

Learning Outcomes

Upon successful completion of this course it is intended that a student will be able to:

- Understand basic concepts of AI and Machine Learning
- Identify applications of AI in chemistry
- Handle simple chemical datasets, Use basic tools for data analysis
- Appreciate the future role of AI in chemical sciences, IPR, scholarly publishing practices, and use of digital tools in scientific communication.

Unit 1 - Introduction to AI (12 Hrs.)

What is AI? Basic definition and importance, Types of AI: Narrow AI, General AI, AI vs Machine Learning vs Deep Learning, Applications of AI in daily life, Role of AI in chemistry.

Unit 2- Basics of Data in Chemistry (12 Hrs.)

Types of chemical data (numerical, spectral, experimental), Data collection and representation, Introduction to datasets, Data cleaning and preprocessing (basic idea), Chemical databases (PubChem, ChemSpider).

Unit 3 - Machine Learning in Chemistry (12 Hrs.)

What is Machine Learning?

Types: (Supervised learning, Unsupervised learning)

Basic concepts: (Training and testing, Features and labels).

Simple examples in chemistry: Predicting boiling point and Classification of compounds

Unit 4 – AI Tools in Chemistry (12 Hrs.)

Introduction to simple tools: (Python basics (very elementary) and Use of Google Colab / simple software). Visualization of chemical data, Use of spreadsheets for data analysis, Introduction to cheminformatics

Unit 5 - Applications of AI in Chemistry (12 Hrs.)

Drug discovery and design, Material science (nanomaterials, catalysts), Environmental chemistry (pollutant detection), Spectral analysis (IR, NMR basics with AI support), Green chemistry and sustainability

Reference Books:

1. Dr. Harsh K. Gaikwad, Dr. Malhari C. Nagtilak, Dr. Priyanka R. Sakhare, Dr. Renukacharya G. Khanapure Role of AI in Drug discovery or in Chemistry, IIP Iterative International Publishers, ISBN: 9789370204225, 9370204229.
2. Eshal Inaaya Saleel. Artificial intelligence in chemistry a comprehensive research in chemistry. 11 A.
3. Dinkar P. Kotwal, Chapter 21: Artificial Intelligence in Chemistry, ISBN: 978-81-957387-4-8.
4. D. Paul *et al.*, Artificial intelligence in drug discovery and development, Drug Discovery Today, (2021)

Websites and eLearning Sources:

1. <https://www.youtube.com/watch?v=D1eL1EnxXXQ>
2. https://www.youtube.com/watch?v=pKeVMlkFpRc&list=PLwdnzlV3ogoXaceHrrFVZCJkbm_laSHcH
3. https://www.youtube.com/watch?v=KMO0pXmsyf4&list=PLFW6lRTa1g82ij-dcyhI_dLSDk_Mb6pR3

COs and Bloom's Taxonomy Mapping – 26CH110

Course Outcomes	On completing U.G. program the students will be able to	BTL
CO1	Explain the fundamental concepts of Artificial Intelligence, Machine Learning, and their relevance to chemistry.	K1
CO2	Identify and interpret different types of chemical data and understand basic data handling techniques.	K2
CO3	Apply basic Machine Learning concepts to simple chemical problems such as prediction and classification.	K3, K4
CO4	Utilize basic computational tools (Python, spreadsheets, Google Colab) for chemical data analysis and visualization.	K5
CO5	Analyze and evaluate the applications of AI in areas such as drug discovery, materials science, and environmental chemistry.	K6

BTL K1 and K2 – remembering and understanding, K3- Applying, K4 – Analyse, K5- Evaluate and K6- Create

Relationship Matrix – 26CH110

Course Outcomes	Programme Outcomes (POs)						Programme Specific Outcomes (PSOs)						Mean Score of Cos
	PO1	PO2	PO3	PO4	PO5	PO6	PSO1	PSO2	PSO3	PSO4	PSO5	PSO6	
CO1	3	2	1	1	1	1	3	1	1	1	1	1	1.4
CO2	3	3	2	1	1	1	3	2	2	1	1	1	1.8
CO3	3	3	3	2	2	1	3	3	2	2	2	2	2.3
CO4	3	3	3	2	2	1	3	3	2	2	2	2	2.3
CO5	3	3	3	3	2	2	3	3	3	3	2	2	2.7
Total													2.1

Mean Score: 3- High, 2- Medium/Moderate, 1-Low

